

5-Methylindan  
874-35-1 | DTXSID5061245

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $2.31 \times 10^{-10}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $3.08 \times 10^{-1}$

**Confidence level:**  $8.31 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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alpha-Phellandrene

**Measured:**  $3.13 \times 10^{-10}$

**Predicted:**  $2.83 \times 10^{-10}$

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alpha-Terpinene

**Measured:**  $3.63 \times 10^{-10}$

**Predicted:**  $2.91 \times 10^{-10}$

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gamma-Terpinene

**Measured:**  $1.77 \times 10^{-10}$

**Predicted:**  $2.06 \times 10^{-10}$

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Cyclohepta-1,3-diene

**Measured:**  $1.39 \times 10^{-10}$

**Predicted:**  $1.35 \times 10^{-10}$

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2,5-Dimethyl-2,4-hexadiene

**Measured:**  $2.10 \times 10^{-10}$

**Predicted:**  $2.11 \times 10^{-10}$